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Advanced Plume Studies

David P. Weaver
Ingrid Wysong
Andrew Ketsdever

AFRL/PRSA
10 E. Saturn Blvd.
Edwards AFB CA 93524-7680

David Campbell
Ghanshyam Vaghjiani
Dean Wadsworth
Angelo Alfano

ERC, Inc.
10 E. Saturn Blvd.
Edwards AFB, CA 93524-7680

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David P. Weaver; Ingrid Wysong; Andrew Ketsdever; David Campbell; Ghanshyam Vaghjiani; Dean Wadsworth; Angelo Alfano

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10 E. Saturn Blvd.
Edwards AFB CA 93524-7680

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10 E. Saturn Blvd.
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AFRL/PRS
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Edwards AFB CA 93524-7048

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14. ABSTRACT
An advanced rarefied gas dynamic capability to simulate plume flow fields, plume surface interactions at high altitudes, and plume chemical mechanisms will provide the AF with the tools to adequately address recent problems critical to several AF programs. A wide variety of intelligence and missile defense applications require high fidelity reacting plume radiation simulations for target tracking and target discrimination (especially in the presence of countermeasures). Developing hypersonic flight and re-entry vehicles can utilize simulations of the nonequilibrium atmospheric shock layer to achieve improved aerothermodynamic performance, propulsion system/vehicle integration, and signature control. Most AF satellite programs require thruster plume/spacecraft interaction (contamination) simulations. In addition, a wide range of AF missions is envisioned for micro- and nano-spacecraft. Micropropulsion is an enabling technology for microspacecraft operations: microspacecraft missions involving large spacecraft resupply, repair or surveillance will require maneuverability. The research necessary to meet AF needs in the plumes and micro-fluids arenas share a scientific basis in rarefied gas dynamic modeling and surface collision physics. Direct simulation Monte Carlo (DSMC) is an important simulation tool for rarefied, nonequilibrium gas flows, including challenging real-world plume cases. This AFRL/PRSA research project develops and applies kinetic and molecular-level models of improved physical realism for nonequilibrium processes such as collisional interaction of gases, gas-particulate mixtures, and gas surface interactions that arise in multi-species, chemically reacting rarefied flowfields such as rocket plumes, thruster contamination, plume-plume and plume-atmosphere interactions and low Reynolds number flows. It also eludicates the chemical mechanisms of UV plume signatures and propellant decomposition.

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FOREWORD

This final report, entitled "Advanced Plume Studies," presents the results of a research study performed under JON 2308M19B by AFRL/PRSA, Edwards AFB CA. The Project Manager for the Air Force Research Laboratory was Dr. Ingrid Wysong.

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INGRID J. WYSONG
Project Manager

________/signed/________________
INGRID J. WYSONG
Chief, Aerophysics Branch

______/signed/__________________
PHILIP A. KESSEL
Technical Advisor
Space & Missile Propulsion Division

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Executive Summary

An advanced rarefied gas dynamic capability to simulate plume flow fields, plume surface interactions at high altitudes, and plume chemical mechanisms will provide the AF with the tools to adequately address recent problems critical to several AF programs. A wide variety of intelligence and missile defense applications require high fidelity reacting plume radiation simulations for target tracking and target discrimination (especially in the presence of countermeasures). Recent interest in the high-altitude Boost-phase Interceptor program has added a particular urgency to this issue. The Space-Based InfraRed System and microsatellite formation programs require thruster plume/spacecraft interaction (contamination) simulations in order to ensure orbit lifetime is not adversely affected and that sensor/solar arrays will not suffer intolerable degradation. Developing hypersonic flight and re-entry vehicles can utilize simulations of the non-equilibrium atmospheric shock layer to achieve improved aerothermodynamic performance, propulsion system/vehicle integration, and signature control.

In addition, a wide range of AF missions is envisioned for micro- and nano-spacecraft. Micropropulsion is an enabling technology for microspacecraft operations: microspacecraft missions involving large spacecraft resupply, repair or surveillance will require maneuverability. Recent developments in silicon chip technology allow for the fabrication of a variety of small-scale propulsion components such as micro-thrusters or micro-valves. These components are vital to the successful development of microspacecraft and many involve microscale fluid flows. The research necessary to meet AF needs in the plumes and micro-fluids arenas share a scientific basis in rarefied gas dynamic modeling and surface collision physics. Direct simulation Monte Carlo (DSMC) is an important simulation tool for rarefied, non-equilibrium gas flows, including challenging real-world plume cases. It will prove to be a key tool, as well, in understanding the gas dynamic and chemical processes associated with the performance and spacecraft interaction effects of micro and nano-propulsion systems. In these micro-fluid flows, the scale of the device begins to approach the mean free path of the molecules, even at atmospheric pressure.

This AFRL/PRSA research project develops and applies kinetic and molecular-level models of improved physical realism for non-equilibrium processes such as collisional interaction of gases, gas-particulate mixtures, and gas surface interaction that arise in high temperature, multi-species, chemically reacting rarefied flowfields such as rocket plumes, plume-plume and plume-atmosphere interactions and low Reynolds number flows. These phenomena are not accurately addressed by standard engineering tools. Lack of a molecular-level understanding of the processes translates into large uncertainties in the prediction of features of the overall flowfield. This, in turn, can result in systems that are exposed to detrimental environments (e.g., contamination of spacecraft optical systems due to deposition of thruster exhaust products), or possess undesirable features (enhanced plume radiative signature of ballistic systems). The key computational tool used in this effort is the Direct Simulation Monte Carlo (DSMC) method. Unique experimental facilities are utilized to provide measurements that indicate key physical principles and provide validation data for the models.

UV signature and propellant decomposition chemistry

The decomposition of energetic hydrocarbons at high heating rate and high temperature was refined to allow gas phase mixtures of hydrocarbons and infrared laser sensitizers to be pyrolyzed and analyzed (gas chromatographically) after a single carbon dioxide laser pulse. These systems were characterized by temperature ramp, maximum temperature, and decomposition mechanism. These experiments refute previously reported results that infrared laser sensitization results in radically different mechanistic branching ratios than those observed in flow reactors for quadricyclanes. The use of IR laser-sensitized pyrolysis for advanced fuel characterization and performance screening has been demonstrated and measurements of the decomposition chemistry of energetic materials have been used to identify key mechanisms that will accelerate the development of new mission-enhancing propellants.

Research into UV radiation chemistry is paving the way for future adoption of UV sensor technology which would provide revolutionary advances in missile defense. Some of the payoffs of UV sensor technology include: higher spatial resolution, lower cost, reduced mass, and improved target discrimination. Experimental data on the fundamental reaction rates and temperature dependencies of gas phase reactions and controlling kinetic mechanisms that produce the radiating species in plumes, such as the CO Cameron bands, were obtained. Specifically, a flash-photolysis apparatus and a discharge flow-tube apparatus were employed to study the gas-phase kinetics of H-atoms, O-atoms and OH radicals with several diamine propellants (e.g. N_2H_4, MMH and UDMH). The reaction rate coefficients were measured as a function of temperature and showed, in all cases, to be independent of pressure in the range studied. Products analysis studies were carried out for the O-atom reactions. Further, a molecular beam experiment was used to determine the nascent excited state product distributions in chemiluminescent reactions, including CH_2 + O. The production of CO(a) and CO(A), both of which are strong UV emitters, by reaction of O with CH was demonstrated. The quenching rate of CO(a) by major plume species has been measured. Thus, a fairly complete picture of the basic science underlying the UV mechanisms relating to hydrazine reactions and CO(a) chemical production has been established and published in the literature.

<u>Non-equilibrium flows, microflows, and contamination</u>

The research necessary to meet AF needs in the plume flows and micro-fluids arenas share a scientific basis in rarefied gas dynamic modeling and surface collision physics. Direct simulation Monte Carlo (DSMC) is an important simulation tool for rarefied, non-equilibrium gas flows, including challenging real-world plume cases. It will prove to be a key tool, as well, in understanding the gas dynamic and chemical processes associated with the performance and spacecraft interaction effects of micro and nano-propulsion systems. In these micro-fluid flows, the scale of the device begins to approach the mean free path of the molecules, even at atmospheric pressure. The results of this project have advanced our basic understanding of rarefied gas flows and the utility of DSMC methods in a number of ways.

The physical models used in DSMC for collision cross sections have been clarified and improved, and studies have included molecular rotational and vibrational relaxation, chemical reactions, and surface collisions. Critical validation data have been provided for gas flowfields, vibrational relaxation data, plume impingement, and nozzle flows. Measurements of an NO freejet expansion flowfield using laser-induced fluorescence were made and showed good agreement with DSMC simulations for density and rotational temperature. Measurements of NO vibrational relaxation rates were made and used to understand the strengths and limitations of simple DSMC relaxation models. DSMC rotational relaxation models were compared in detail with the best experimental and theoretical results from the literature, and guidelines for usage recommended. A variety of DSMC chemical reaction models were compared and elucidated, with particular emphasis on the role of vibrational favoring effects. Further, the critical role of the collision selection algorithm and the total collision cross section were clarified.

A number of studies were completed concerning contamination of spacecraft via thruster interactions. A fiberoptic sensor was developed and tested to monitor ion sputtering. Forces from nozzle backflows were measured, as well as interactions between multiple jet flows and plumes onto surfaces.

Gas-surface interaction models currently used for DSMC are highly simplified, and represent an important uncertainty in most rarefied gas dynamic simulations. The general gas-surface interaction (GSI) event is considered to be parameterized by the molecule's incident energy magnitude and incident angle relative to the surface normal. These parameters are used to estimate the degree of non-equilibrium that arises for typical applications and the quality of scattering predictions made by common few-parameter models such as the Maxwell model. Experimental measurements and molecular dynamics simulations have been evaluated as potential sources of data to develop and/or test improved models. An ad hoc model was used to quantify the effect that improved physical realism of non-equilibrium scattering events may have on typical surface quantities of interest for applications in the rarefied regime.

A specific implementation of micro-fluid flows and micropropulsion research was the design and optimization of the Free Molecular MicroResistojet (FMMR) thruster for spacecraft propulsion. The FMMR was designed as a micropropulsion system capable of performing attitude control and primary

maneuvers for nanospacecraft with mass less than 10 kg. The FMMR is constructed using microelectromechanical systems (MEMS) fabrication techniques, which allows it to be machined on a micrometer scale and to be easily integrated with other MEMS components such as embedded control systems, valves, and pressure regulators. The details of gas-surface interactions between propellant molecules and surfaces held at elevated temperature are critical in predicting the propulsion system's performance and efficiency. A parametric assessment was made of the performance of a typical thruster geometry using a general Maxwell scattering model and two versions of the Cercignani-Lampis-Lord model. The models are incorporated into a Direct Simulation Monte Carlo numerical code and are used to bound the predicted performance characteristics of the thruster. The total specific impulse varies by approximately 20% over range of accommodation coefficients from specular to diffuse surface scattering.

For thruster systems which utilize gas expansion through micronozzle geometries, the operation of low Reynolds number gas expansions are required. Cold gas flows have been compared for a thin-walled, underexpanded orifice and a conical nozzle as a function of Reynolds number. The range of Reynolds numbers investigated range from below 1 to nearly 400. The nozzle thrust to orifice thrust ratio was found to be below unity for Reynolds numbers below 70 for helium, argon and nitrogen propellants. For a thrust ratio below unity, the orifice has a higher propulsive efficiency when compared to the conical nozzle. The thrust data is shown to transition from a free molecule solution at the low thrust range to nearly the continuum, inviscid solution at the high thrust range. Thrust data was obtained for the same nozzle geometry over almost four orders of magnitude in thrust. This represents the first known data to directly compare a conical nozzle geometry to the relatively simple orifice geometry.

The ability to measure extremely low thrust levels with unusual precision is becoming more critical as attempts are made to characterize the performance of emerging micropropulsion systems. Many new attitude control concepts for nanospacecraft involve the production of thrust below 1 μN. A simple, but uniquely successful thrust stand has been developed and used to measure thrust levels as low as 90 nano-Newtons with an estimated accuracy of 11%. Thrust levels in the range of 712 nN to 1 μN have been measured with an estimated accuracy of 2%. Thrust is measured from an under expanded orifice operating in the free molecule flow regime with helium, argon, and nitrogen propellants. The thrust stand is calibrated using results from direct simulation Monte Carlo numerical models and analytical solutions for free molecule orifice flow. The accuracy of the gas dynamic calibration technique, using free molecule orifice flow, has also been investigated. It is shown that thrust stand calibration using high Knudsen number helium flow can be accurate to within a few percent in the 80 to 1 μN thrust range for thin walled orifices when the stagnation pressure is accurately measured.

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